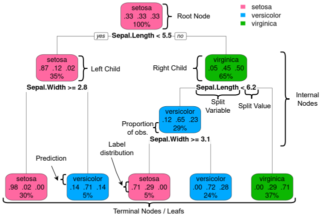
Introduction to Machine Learning

CART

In a nutshell



Learning goals

- Understand basic structure of CART models
- Understand basic concepts used to fit CART models

LEARNING AND PREDICTION WITH CARTS

Training

Input: Labeled data

Sepal Width	Sepal Length	Species
3,5	5,1	Setosa
3,0	5,9	Virginica
2,5	6,3	Virginica
2,2	6,2	Versicolor

Tree Learner

Output

Tree Model

Prediction

Input: Unlabeled data

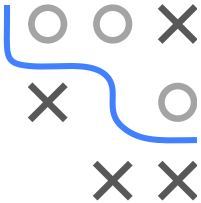
Sepal Width	Sepal Length	Species
3,0	7,7	?
3,1	6,9	?
2,3	6,3	?
3,0	5,6	?

Tree Model

Prediction

Level of Happiness
Setosa
Versicolor
Virginica
Versicolor

WHAT IS A TREE?



Basic idea:

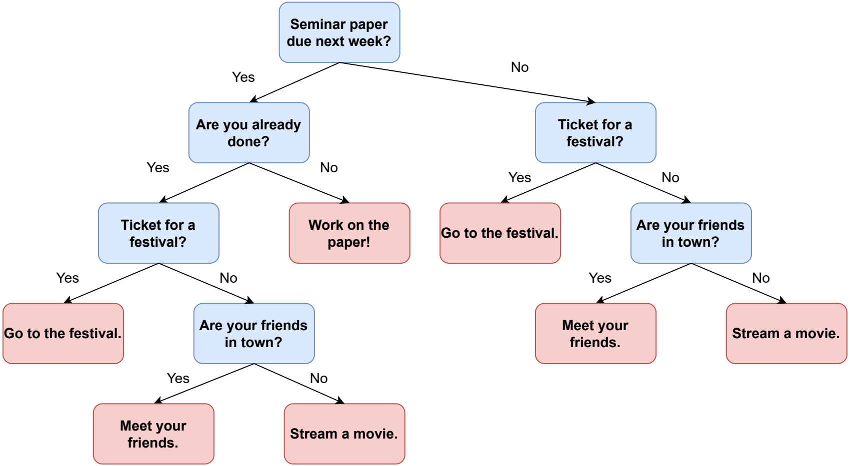
- Divide feature space into sub-regions.
- For each region, learn best constant prediction from training data.

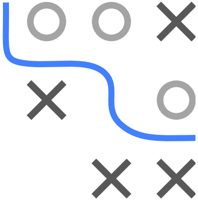
Classification **A**nd **R**egression **T**rees are a class of models that can:

- model non-linear feature effects
- facilitate interactions of features
- be inherently interpreted

WHAT IS A TREE?

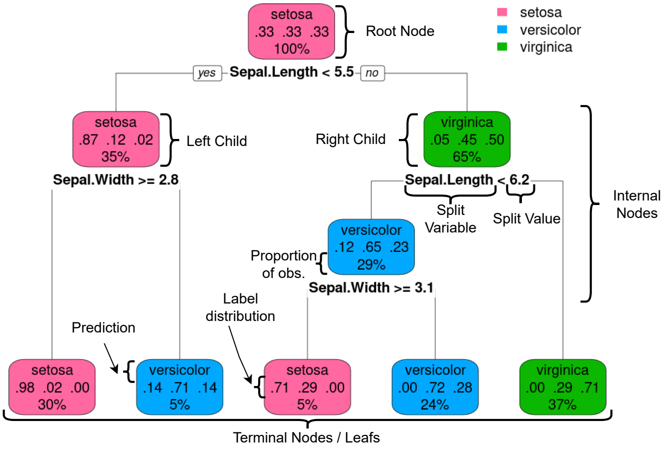
A decision tree is a set of hierarchical binary partitions, e.g., your evening planning decision (target) could be based on a decision tree:





WHAT IS A TREE?

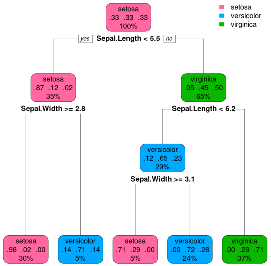
Instead of life choices, we can predict the `Species` of flowers described in the `iris` data set using features `Sepal.Width` and `Sepal.Length`.

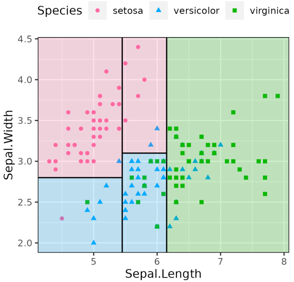


CART AS A PREDICTOR

Instead of the visual description, we can also describe trees through their division of the feature space $\mathcal{X}$ into **rectangular regions**, Q_m:

$$f(\mathbf{x}) = \sum_{m=1}^{M} c_m \mathbb{I}(\mathbf{x} \in Q_m),$$

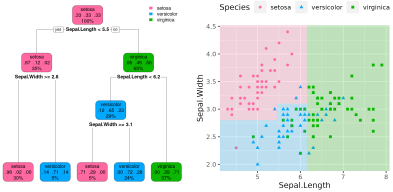




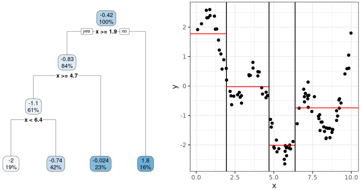
TASKS FOR CART

- CARTs can have categorical and numerical targets.
- In both cases, the leafs, i.e., the ultimate nodes, define the predictions.

Categorical target:



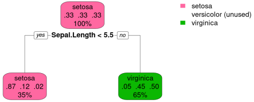
Numerical target:

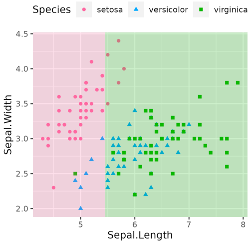


HOW TO FIT A CART

- A *recursive* greedy search in the feature space optimizes CARTs
- In each iteration, the best split is selected

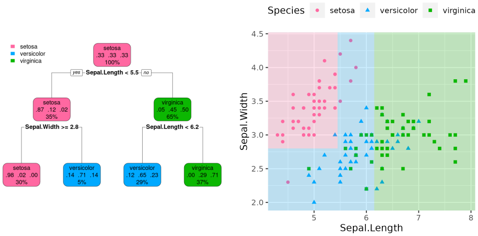
Iteration 1:



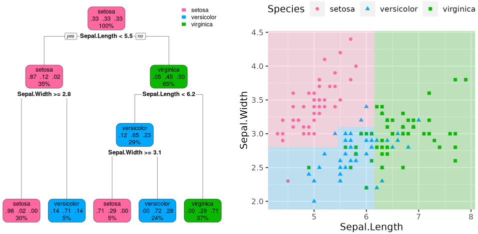


HOW TO FIT A CART

Iteration 2:

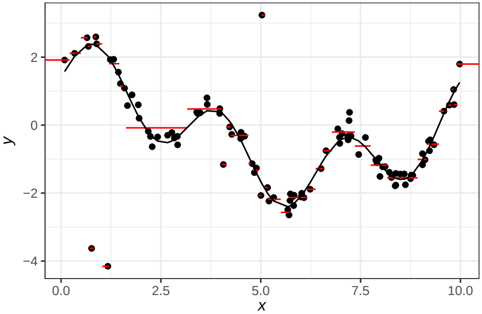


Iteration 3:



HOW TO FIT A CART

- This procedure can run until each observation has its own leaf.
- Then, the tree will not generalize well and overfit:



- Thus, we need techniques to keep the tree small and informative.

⇒ In practice, trees are often used as base learners for ensemble learners like Random Forests.